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The Padé Approximant*

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We present a method in which the Padé approximant is used to calculate the asymptotic behavior of a function from the first few terms of its power series. We illustrate this method by two examples and give a partial justification of it. One of the examples is a calculation of the binding energy of a Fermi gas of hard spheres.

I. INTRODUCTION

The Padé approximant is well known in mathematics [1].[1] This paper contains two examples of the application of the method to problems in mathematical physics. Both examples consist of rearrangements of infinite series for large values of the expansion parameter (possibly even values of the expansion parameter for which a series diverges), yet useful results are obtained by using only the first few terms of the series.

In the last section we discuss the proof of the validity of these procedures. The basic result is, if $f(z)$ goes to infinity like z^k, then the $[p, p+k]$ Padé approximants converge to the correct coefficient of z^k in the limit as p goes to infinity.

II. THE SCATTERING LENGTH OF A HARD CORE POTENTIAL

The first two terms in the iterated solution of the integral equation for the K-matrix are

$$(\mathbf{k}'|K|\mathbf{k}) = (\mathbf{k}'|V|\mathbf{k}) - \frac{1}{2\pi^2}\int d\mathbf{k}'' \frac{(\mathbf{k}'|V|\mathbf{k}'')(\mathbf{k}''|V|\mathbf{k})}{k''^2 - k^2} \tag{1}$$

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[1] We follow the notation of reference 1.

where

$$(\mathbf{k}'|V|\mathbf{k}) = \frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\mathbf{r} \exp(-i\mathbf{k}'\cdot\mathbf{r})V(r)\exp(i\mathbf{k}\cdot\mathbf{r}) \tag{2}$$

and the scattering length is

$$a = -(0|K|0) \tag{3}$$

For the repulsive square well potential

$$(\mathbf{k}|V|0) = \frac{2\mu V}{\hbar^2} c^3 \left[\frac{\sin kc}{(kc)^3} - \frac{\cos kc}{(kc)^2}\right] \tag{4}$$

so that

$$a = -\frac{1}{3}g + \frac{2}{\pi}g^2\frac{1}{c}N \tag{5}$$

where

$$g = \frac{2\mu V}{\hbar^2}c^3$$

$$N = \int_0^\infty dx \left[\frac{\sin x}{x^3} - \frac{\cos x}{x^2}\right]^2 = \frac{\pi}{15} \tag{6}$$

$$x = k''c$$

For $V \to +\infty$, a will be finite; therefore, we replace Eq. (5) by the [1,1] Padé approximant

$$a = -\frac{1}{3}g \bigg/ \left(1 + \frac{6}{\pi}g\frac{N}{c}\right) \tag{7}$$

$$\to -\frac{5}{6}c \qquad \text{for } g \to \infty$$

This last result may be compared with the exact result

$$a = -c \tag{8}$$

It is possible to answer the question of the convergence of the sequence of Padé approximants to a itself more sharply. There is an exact result corresponding to Eq. (5); namely

$$a = -c + c\frac{\tanh\sqrt{g/c}}{\sqrt{g/c}} \tag{9}$$

which may be derived from elementary considerations (solving the Schrödinger equation for a repulsive square well by fitting boundary conditions). By expanding Eq. (9) in powers of g, it is possible to find any of the sequence of Padé approximants [1,1], [2,2], [3,3],.... The result of a number of such calculations is shown in Table I.

TABLE I

Padé approximant a		Fredholm approximant a	
[1,1]	$-5/6\,c$	[1,1]	$-2/3\,c$
[2,2]	$-14/15\,c$	[2,2]	$-4/5\,c$
[3,3]	$-27/28\,c$	[3,3]	$-6/7\,c$
[4,4]	$-44/45\,c$	[4,4]	$-8/9\,c$

The Fredholm series is, obviously,

$$a = -c + c\,\frac{\sinh\sqrt{g/c}/\sqrt{g/c}}{\cosh\sqrt{g/c}} \tag{10}$$
$$= -c + c\,\frac{1 + \dfrac{1}{6}\dfrac{g}{c} + \dfrac{1}{120}\dfrac{g^2}{c^2} + \dots}{1 + \dfrac{1}{2}\dfrac{g}{c} + \dfrac{1}{24}\dfrac{g^2}{c^2} + \dots}$$

from which we may form a sequence of "Fredholm approximants" in an obvious way. The results are also shown in Table I.

In our second example, an integral similar to N (Eq. (6)) appears which cannot be evaluated by elementary methods. It is possible to compute the value of N using the Padé approximant method as follows. If we expand

$$\left[\frac{\sin x}{x^3} - \frac{\cos x}{x^2}\right]^2 = \alpha + \beta\, x^2 + \gamma x^4 + \dots$$
$$\alpha = \frac{1}{9}, \qquad \beta = -\frac{1}{45}, \qquad \gamma = \frac{1}{525}, \dots \tag{11}$$

we must cut off the integral at an upper limit K to integrate term by term. Since N is finite as K goes to infinity, we form a modified Padé approximant as follows

$$N = \alpha K\left(1 - \frac{2}{3}\frac{\beta}{\alpha}K^2\right)^{-1/2} \tag{12}$$

The limit $K \to \infty$ is evaluated by calculating the value of the modified Padé approximant at the magnitude of the first pole of its denominator.[2] We find

$$\frac{2}{\pi} N \to \frac{\alpha}{\pi} \left(- \frac{1}{3} \frac{\beta}{\alpha} \right)^{-1/2} = 0.13697877 \tag{13}$$

which may be compared with the exact result

$$\frac{2}{\pi} N = \frac{2}{15} = 0.13333333 \tag{14}$$

III. The Energy of a Fermi Gas of Hard Spheres

We start with a repulsive square well potential of radius c and "depth" V. The first two terms in the iterated solution of Brueckner's K-matrix equation are

$$(\mathbf{k}'|K(\mathbf{p})|\mathbf{k}) = (\mathbf{k}'|V|\mathbf{k}) - \frac{1}{2\pi^2} \int d\mathbf{k}'' \frac{(\mathbf{k}'|V|\mathbf{k}'')(\mathbf{k}''|V|\mathbf{k})}{k''^2 - k^2} \tag{15}$$

Because of the exclusion principle, the integral is restricted to run over k''

$$\begin{aligned} |\tfrac{1}{2}\mathbf{p} + \mathbf{k}''| &> k_F \\ |\tfrac{1}{2}\mathbf{p} - \mathbf{k}''| &> k_F \end{aligned} \tag{16}$$

where k_F is the Fermi momentum. We are using unmodified energy denominators because we want the energy of the system only up to order V^2. We assume that the K-matrices are relatively independent of the total momentum $\mathbf{p}$ of the interacting pair and substitute $\mathbf{p} = 0$ everywhere.

We need only the diagonal elements ($\mathbf{k}' = \mathbf{k}$) of K and the exchange terms ($\mathbf{k}' = -\mathbf{k}$). The integral in Eq. (20) may be evaluated in the same way as N was evaluated by a Padé method in our previous example; namely, by expanding the potential matrix elements in powers of c. It is again necessary to cutoff at an upper limit K; we shall let $K \to \infty$ *after calculating the total energy of the system* by forming a Padé approximant to the total energy which remains finite as $K \to \infty$. We find

[2] We expect to discuss the validity of this procedure for functions with essential singularities at ∞ in a subsequent publication. Since $N(z)$ has no poles in the finite plane, the Padé approximant cannot represent N past its first pole; therefore, the magnitude of the first pole is as far as we can proceed toward infinity.

$$I \equiv \frac{1}{2\pi^2} g^2 \int d\mathbf{k}'' \left[\frac{1}{3} - \frac{1}{30} |\mathbf{k}' - \mathbf{k}''|^2 c^2\right]\left[\frac{1}{3} - \frac{1}{30} |\mathbf{k} - \mathbf{k}''|^2 c^2\right] \Big/ k''^2 - k^2$$

$$= \frac{1}{2\pi^2} g^2 \int d\mathbf{k}'' \left[\frac{1}{9} - \frac{1}{45} (k^2 + k''^2 - kk''\mu \mp kk''\mu) c^2\right] \Big/ k''^2 - k^2 \qquad (17)$$

where μ is the cosine of the angle between $\mathbf{k}''$ and $\mathbf{k}$. (The $-$ sign for $\mathbf{k}' = \mathbf{k}$; the $+$ sign for $\mathbf{k}' = -\mathbf{k}$; however, this term vanishes upon integration anyway)

$$I = \frac{2}{\pi} g^2 \int_{k_F}^{K} dk'' \frac{k''^2}{k''^2 - k^2} \left[\frac{1}{9} - \frac{1}{45} (k^2 + k''^2) c^2\right] \qquad (18)$$

We make use of tables [2] of elementary integrals to obtain

$$I = \frac{2}{\pi} g^2 \left[\left(\frac{1}{9} - \frac{c^2}{45} k^2\right)\left(K - \frac{k}{2} \ln \left|\frac{K+k}{K-k}\right| - k_F + \frac{k}{2} \ln \left|\frac{k_F + k}{k_F - k}\right|\right)\right.$$
$$\left. - \frac{c^2}{45}\left(\frac{K^3}{3} + k^2 K - \frac{k^3}{2} \ln \left|\frac{K+k}{K-k}\right| - \frac{k_F^3}{3} - k^2 k_F + \frac{k^3}{2} \ln \left|\frac{k_F + k}{k_F - k}\right|\right)\right] \qquad (19)$$

The terms with $\ln |(K + \mathbf{k})/(K - \mathbf{k})|$ have a finite limit as $K \to \infty$, namely zero, so we drop them immediately.

As previously stated, we will not form a Padé approximant to take the limit $K \to \infty$ at this point; rather, we will calculate the total energy of the system first and then make a Padé approximant.

The potential energy of the system is

$$\frac{M}{\hbar^2} V = \frac{1}{2} \frac{1}{2\pi^2} \int d\mathbf{m} \int d\mathbf{n}\, [4(\mathbf{mn}|K|\mathbf{mn}) - (\mathbf{nm}|K|\mathbf{mn})] \Big/ \int d\mathbf{m} \qquad (20)$$

Since the K matrices do not depend on p, we use as variables

$$\begin{aligned} \mathbf{m} + \mathbf{n} &= \mathbf{p} \\ \tfrac{1}{2}(\mathbf{m} - \mathbf{n}) &= \mathbf{k} \end{aligned} \qquad (21)$$

The Jacobian of this transformation is 1. We integrate over the $\mathbf{p}$'s such that

$$\begin{aligned} |\tfrac{1}{2}\mathbf{p} + \mathbf{k}| &< k_F \\ |\tfrac{1}{2}\mathbf{p} - \mathbf{k}| &< k_F \end{aligned} \qquad (22)$$

to find

$$\frac{M}{\hbar^2} V = \frac{1}{2} \frac{(4\pi)^2}{2\pi^2} \int_0^{k_F} k^2\, dk \left(\frac{8}{3} k_F{}^3 - 4k_F{}^2 k + \frac{4}{3} k^3 \right) \tag{23}$$

$$\times \left(3\frac{g}{3} + \frac{g}{30} (2kc)^2 - 3I \right) \Big/ \frac{4\pi}{3} k_F{}^3$$

The terms in the last parenthesis in Eq. (23) arise in the following way:

$$(\mathbf{k}|V|\mathbf{k}) = \frac{g}{3}$$

$$(-\,\mathbf{k}|V|\mathbf{k}) = \frac{g}{3} - \frac{g}{30} (2kc)^2 + \dots$$

$$\therefore\ (\mathbf{k}|K|\mathbf{k}) = \frac{g}{3} - I \tag{24}$$

$$(-\,\mathbf{k}|K|\mathbf{k}) = \frac{g}{3} - \frac{g}{30} (2kc)^2 - I$$

$$\therefore\ 4(\mathbf{k}|K|\mathbf{k}) - (-\,\mathbf{k}|K|\mathbf{k}) = (\text{last parenthesis})$$

In spite of the complicated appearance of I as given by Eq. (19), all of the integrals in Eq. (23) are elementary:

$$\int_0^{k_F} k^n\, dk \ln \frac{k_F + k}{k_F - k} = A_{n+1}\, k_F{}^{n+1} \tag{25}$$

where the A's are [3]

$$A_m = m^{-1} \left[(1 - (-1)^m) \log 2 + \sum_{\nu=1}^{m} (1 - (-1)^{m-\nu})/\nu \right] \tag{26}$$

We find

$$\frac{MV}{\hbar^2} = \frac{3k_F{}^3}{\pi} \left[g \left\{ \frac{1}{9} + \frac{k_F{}^2 c^2}{225} \right\} - \frac{g^2}{3\pi} \left\{ k_F \left(\frac{222}{315} - \frac{128}{105} \log 2 \right) + \right. \right. \tag{27}$$

$$\left. \left. c^2 k_F{}^3 \left(\frac{118}{567} - \frac{64}{189} \log 2 \right) + K \left(\frac{2}{9} - \frac{2c^2 k_F{}^2}{75} \right) - \frac{2c^2 K^3}{135} \right\} \right]$$

First, we make a modified [1, 0] Padé approximant to the terms with K and K^3 to find the limit as $K \to \infty$. We find in the same manner as in Eq. (13)

$$\alpha K + \beta K^3 \approx \alpha K \sqrt{1 + 2\beta K^2/\alpha} \approx \frac{\alpha K}{\sqrt{1 - 2\beta K^2/\alpha}} \to \sqrt{-\frac{\alpha^3}{4\beta}}$$
$$\lim_{K\to\infty} (\alpha K + \beta K^3) \to \left[15\left(1 - \frac{3}{25} k_F{}^2 c^2\right)^3\right]^{1/2} \Big/ 9c \tag{28}$$

Finally, we make a [1,1] Padé approximant to

$$ag - bg^2 \to \frac{ag}{1 + bg/a} \to a^2 b \qquad \text{as} \qquad g \to \infty \tag{29}$$

where

$$a = 1/9 + k_F{}^2 c^2/225 \tag{30}$$

$$b = \frac{1}{3\pi}\left\{15\left(1 - \frac{3}{25} k_F{}^2 c^2\right)^3\right]^{1/2} \Big/ 9c - k_F(.14021752 + 0.038339456\, c^2 k_F{}^2)\right\}$$

$$\frac{MV}{\hbar^2} \to 3k_F{}^3 a^2/(\pi b)$$

We may compare this expression with results derived by other methods. We find to order c^2,

$$\frac{MV}{\hbar^2} = \frac{k_F{}^3 c}{\pi}\left(\frac{\pi}{\sqrt{15} - 1.2619577\, k_F c}\right) \approx \frac{k_F{}^3 c}{\pi} (0.811155 + 0.2640344\, k_F c) \tag{31}$$

whereas the exact result to this order is [4]

$$\frac{MV}{\hbar^2} = \frac{k_F{}^3 c}{\pi} (1 + 0.5246\, k_F c) \tag{32}$$

The error in the first term of Eq. (31) corresponds exactly to the error 5/6 in the scattering length calculation since the Lenz term comes entirely from the upper limit.

Our expression Eq. (31) for V is infinite for $r_0 \approx 0.6\, c$. This is reasonable in view of the fact that the density of the system cannot exceed some such limit.

IV. The Padé Theorem

If we have a function represented by a power series about the origin and we know that it goes to infinity like z^k, then the sequence of Padé approximants $[p, p+k]$ converge so that

$$\lim_{p\to\infty} \lim_{z\to\infty} [p, p+k]/f(z) = 1 \tag{33}$$

While we cannot give a completely rigorous proof of this result, we can give a sufficiently detailed discussion to make (38) appear to be true for at least a certain class of $f(z)$ and to illuminate the nature of the Padé approximant.[3] We restrict our discussion to the case $k = 0$, for simplicity. The case $k \neq 0$ can be reduced to the $k = 0$ case suitable manipulations.

Let us consider $f(z)$ regular except for poles such that there exists a series of contours going to infinity on which $|f(z)| < L$. Then we must have [6]

$$f(z) = f(0) + \sum_{n=1}^{\infty} \left(\frac{b_n}{a_n - z} - \frac{b_n}{a_n} \right) \tag{34}$$

If we also assume $\Sigma_{n=1}^{\infty} |b_n/a_n|$ converges then

$$f(z) = A + \sum_{n=1}^{\infty} \frac{b_n}{a_n - z} \tag{35}$$

Let the $|a_n|$ be ordered. Thus for

$$0 \leqslant |z| < |a_1| \leqslant |a_2| \leqslant \dots \leqslant |a_n| \leqslant \dots \tag{36}$$

we may expand and reverse the order of summation

$$f(z) = A + \sum_{m=0}^{\infty} \left(\sum_{n=1}^{\infty} b_n \, a_n^{-(m+1)} \right) z^m \tag{37}$$

[3] Recently, Lu Ke [5] has proved for a different class of functions than we are considering that $\lim_{p\to\infty} \{[p, p] - f(z)\} = 0$ except where $f(z)$ is singular or cut and the point $z = \infty$. He also gives explicit formulas for the $[p, p]$ Padé approximants for this class of functions.

To obtain the $[N, N]$ Padé approximant for $f(z)$, we note that if

$$f(z) = \sum_{j=0}^{\infty} f_j z^j, C(z) = \sum_{j=0}^{\infty} c_j z^j, D(z) = \sum_{j=0}^{\infty} d_j z$$
$$f(z)D(z) - C(z) = 0(z^{2N+1}) \tag{38}$$

then part of the equations for the coefficients are

$$\begin{bmatrix} f_N & f_{N-1} & f_{N-2} & \cdots & f_1 & f_0 \\ f_{N+1} & f_N & f_{N-1} & \cdots & f_2 & f_1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ f_{2N} & f_{2N-1} & f_{2N-2} & \cdots & f_{N+1} & f_N \end{bmatrix} \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} c_N \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{39}$$

By Cramer's rule for solving linear equations we easily find

$$A_N = \lim_{z \to \infty} \frac{C(z)}{D(z)} = \frac{c_N}{d_N} = \frac{\det \begin{vmatrix} f_0 & f_1 & \cdots & f_N \\ f_1 & f_2 & \ddots & \vdots \\ \vdots & & & \vdots \\ f_N & & \cdots & f_{2N} \end{vmatrix}}{\text{cofactor of } f_0} \tag{40}$$

If β_n and α_n are the residues and locations of the poles of the $[N, N]$ Padé approximant, then we find, in a manner similar to the derivation of Eq. (37), that they satisfy the equations

$$\sum_{n=1}^{N} \beta_n \alpha_n^{-m-1} = f_m, m = 1, \ldots, 2N \tag{41}$$

If we define $\tau_j(N)$ as $(-1)^j$ times the jth symmetric function of the $\alpha_n(\tau_0(N) = 1)$ and multiply the jth row of the numerator of (40) by $\tau_j(N)$ and add all these products to the zeroth row, then all but the first term is zero as

$$\sum_{j=0}^{N} \tau_j(N) \alpha_n^{k-j} = 0 \tag{42}$$

since Eq. (42) is the characteristic polynomial of the α_n^{-1}. We then obtain

$$A_N = A + \left(\sum_{n=1}^{\infty} b_n/a_n - \sum_{n=1}^{N} \beta_n/\alpha_n \right) \tag{43}$$

We expect the term in parenthesis to go to zero as $N \to \infty$. Consider $M < N$ such that $|a_M| < |a_{M+1}|$. Then, if N is large enough we may make

$$|a_M|^N \sum_{n=M+1}^{\infty} b_n/a_n^N \tag{44}$$

as small as we please so that the $m = 2N - 2M + 1, \ldots 2N$ equations will determine β_n, α_n, $n \leqslant M$, as closely as we like. The remaining $N - M$ poles will be determined with varying accuracy. Over all we would not expect the error in (43) to be larger than, say, some constant times $\Sigma_{n=N+1}^{\infty} |b_n/a_n|$ and so it tends to zero as N tends to infinity.

From our analysis, we see that the $[N, N]$ Padé approximately reproduces the closest N poles in the rational fraction expansion of $f(z)$. If the poles recede rapidly, as they do in the scattering length example, then the approximation becomes good quickly.

IV. Conclusion

The idea has many applications. For example, it is usually asserted that the no distortion approximation (as used in the $n - d$ scattering problem, for example) is not applicable to potentials with hard cores. But obviously we can calculate the no distortion approximation for a weakly repulsive core and find the first two terms in a power series expression (say for the $n - d$ quartet scattering length) and pass to the limit of an infinitely repulsive core by forming a Padé approximant

$$\alpha V - \beta V^2 = \frac{\alpha V}{1 + \frac{\beta}{\alpha} V} \to \frac{\alpha^2}{\beta}$$

(A finite potential exterior to the core can be carried in the calculation.) In such a problem, it is probably possible to prove that the procedure is correct and to ascertain the degree of approximation for a low order Padé approximant.

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